Toward an Automated-Algebra framework for Quantum Matter with the Quantum Virial Expansion and beyond

Yaqi Hou

S@INT Seminars, Seattle
Sep. $22^{\rm th}$, 2022

Computational Quantum Matter Group

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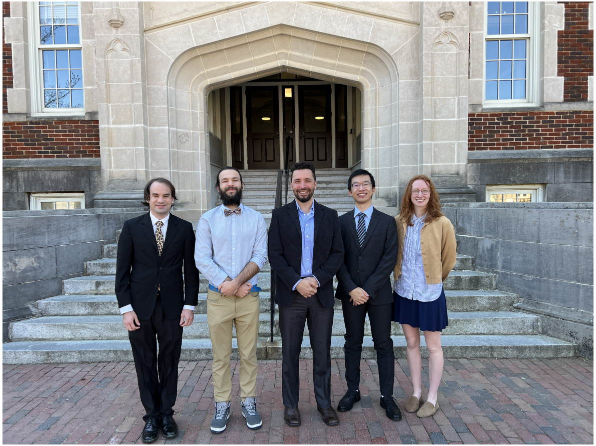

(Left to Right) Andrew Loheac, Aleks Czejdo, Joaquin Drut, Me and Kaitlyn Morrell

Undergraduates:
Austin Blitstein
Kean Leung

Before we start. . .

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The good, the bad and the ~~ugly~~ beautiful (Claim of this talk)

1. The "automated algebra" is promising and there is untapped potential following this direction
2. AA is unfortunately limited (still useful) due to the computational wall
3. Tried to avoid being overly technical, but inevitably somewhat technical

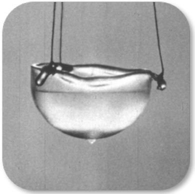
The Devil's Dictionary

Automated Algebra	the thing making this talk coming true
Quantum Virial Expansion	a term with confusing ambiguity
Quantum Matter	our ticket to the party

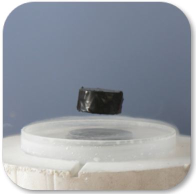
Fermionic many-body systems

CMP

Ultracold atom



Superfluid

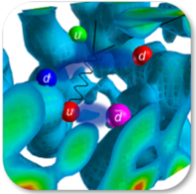


Superconductor

NP

Neutron star

Nuclear matter



QCD Matter

Fermionic many-body systems

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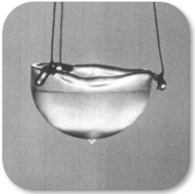

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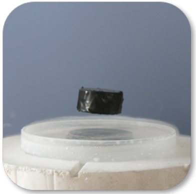

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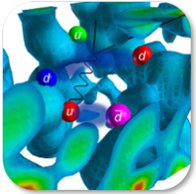


QCD Matter

Ultracold Atoms

Properties of interest

- Experimentally accessible

  the well-known laser trapping and cooling techniques
- Highly tunable

  coupling strength, polarization, dimension, etc.
- Clean and simple

  non-relativistic, dilute spin-1/2 fermions

Hamiltonian

We consider exclusively the non-relativistic, contact interaction model

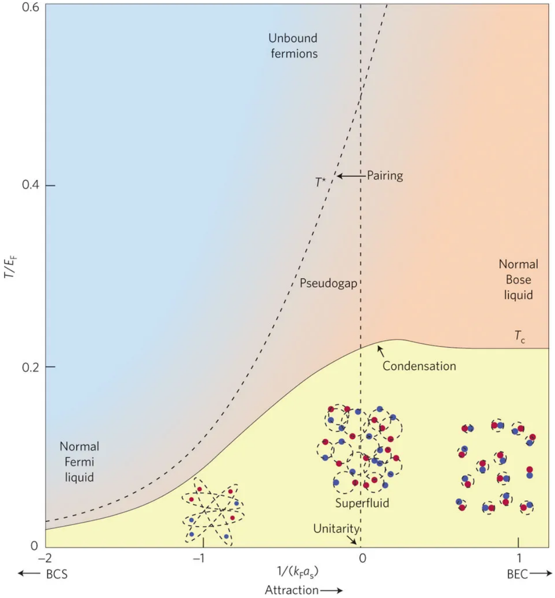
$$\hat{H} = \hat{T} + \hat{V} + \hat{V}_{\text{ext}}$$

- Non-relativistic

$$\hat{T} = \int \mathrm{d}\mathbf{p}\, \frac{\mathbf{p}^2}{2m} \left[\hat{n}_{\uparrow}(\mathbf{p}) + \hat{n}_{\downarrow}(\mathbf{p})\right]$$

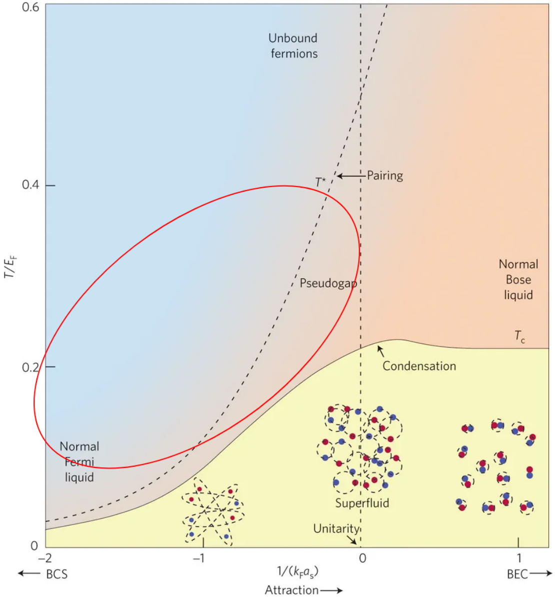
- Contact interaction

$$\hat{V} = -g \int \mathrm{d}\mathbf{x}\; \hat{n}_{\uparrow}(\mathbf{x})\hat{n}_{\downarrow}(\mathbf{x})$$



BCS-BEC crossover (3D) Phase Diagram

Randeria
Nature Phys., **6**, 561–562 (2010)



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BCS-BEC crossover (3D) Phase Diagram

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Overview

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1. Review of Quantum Virial Expansion
2. Introduction of Automated-Algebra method
3. Homogeneous Systems
   - Unitary Fermi Gas
   - General dimension and coupling strength
4. Harmonically Trapped System
   - General dimension and coupling strength (*)
5. Summary, outlook, and ongoing works

Line of Research

Hou, Czejdo, DeChant, Shill and Drut, PRA **100**, 053627 (2019)
Hou and Drut, PRL **125**, 050403 (2020) - UFG
Hou and Drut, PRA **102**, 033319 (2020) - UFG & General dimension
Hou, Morrell, Czejdo and Drut , PRR **3**, 033099 (2021) - Trapped system
Czejdo, Drut, Hou and Morrell, Condensed Matter **7**, 13 (2022) - Review

Spinoff

Czejdo, Drut, Hou, McKenney and Morrell, PRA **101**, 063630 (2020)
Rammelmüller, Hou, Drut and Braun, PRA **103**, 043330 (2021)

Quantum Virial Expansion

Quantum virial expansion is an expansion in powers of fugacity z

$$-\beta\Omega = \ln \mathcal{Z} = Q_1 \sum_{n=1}^{\infty} z^n b_n$$

$z = \exp(\beta\mu)$ - fugacity

Ω - grand potential

b_n - n^{th} order virial coefficient

The grand-canonical partition function is

$$\mathcal{Z} = \mathrm{Tr}_F[\mathrm{e}^{-\beta(\hat{H}-\mu\hat{N})}] = \sum_{n=0}^{\infty} z^n Q_n$$

$\beta = 1/(kT)$ - inverse temperature

Q_n - canonical n-particle partition function

Quantum Virial Expansion

First few b_ns

$$b_1 = 1$$

$$b_2 = \frac{Q_2}{Q_1} - \frac{Q_1}{2!}$$

$$b_3 = \frac{Q_3}{Q_1} - b_2 Q_1 - \frac{Q_1^2}{3!}$$

$$b_4 = \frac{Q_4}{Q_1} - \left(b_3 + \frac{b_2^2}{2}\right) Q_1 - b_2 \frac{Q_1^2}{2!} - \frac{Q_1^3}{4!}$$

For formulas of higher-order terms:
Hou, Czejdo, DeChant, Shill and Drut, Phys. Rev. A **100**, 053627 (2019)

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Interesting facts about b_n

- b_n is directly related to the Q_n
- b_n is dimensionless & volume-independent
- b_n is a universal constant at unitarity

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Quantum Virial Expansion

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Non-interacting b_n in d homogeneous spatial dimensions

$$b_n^{(0)} = \frac{(-1)^{n+1}}{n^{d/2+1}}$$

For formulas of higher-order terms:
Hou, Czejdo, DeChant, Shill and Drut, Phys. Rev. A **100**, 053627 (2019)

Quantum Virial Expansion

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First few b_ns

$$\begin{aligned}\Delta b_1 &= 0\\ \Delta b_2 &= \frac{\Delta Q_2}{Q_1}\\ \Delta b_3 &= \frac{\Delta Q_3}{Q_1} - Q_1 \Delta b_2\\ \Delta b_4 &= \frac{\Delta Q_4}{Q_1} - \Delta\left(b_3 + \frac{b_2^2}{2}\right) Q_1 - \frac{\Delta b_2}{2} Q_1^2\end{aligned}$$

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Quantum Virial Expansion

History of Δb_n

- Second order: Δb_2
  analytically given by Beth-Uhlenbeck formula (1937)
  (1D, 2D, 3D, arbitrary coupling)

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History of Δb_n

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- Third order: Δb_3

  numerical methods (2000s-2010s)

  Path Integral Monte Carlo, sum-over-states, complex Langevin, ...

  See also Larsen, S. Y. et al. Ann. Phys., **374**, 291-313 (2016) for a generalization of Beth-Uhlenbeck formula to three-body problem.

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- Beyond: Δb_n

  very few numerical attempts at Δb_4, nothing beyond

  solving $n-$particle system for large n is hard

  limited to unitarity (i.e. all in 3D only)

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METHODOLOGY (THE UGLY/BEAUTIFUL)

Automated-algebra method

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Expression to evaluate

The n-body physics is encoded in b_n, which depends on Q_N

$$Q_N = \mathrm{tr}_N[\mathrm{e}^{-\beta \hat{H}}]$$

Automated-algebra method

Expression to evaluate

The n-body physics is encoded in b_n, which depends on Q_N

$$Q_N = \mathrm{tr}_N[\mathrm{e}^{-\beta\hat{H}}]$$

Discretize imaginary time with relative small N_τ

$$Q_N = \mathrm{tr}_N\left[\exp\left(-\beta\hat{H}\right)\right] \simeq \mathrm{tr}_N\left[\prod^{N_\tau}\exp\left(-\tau\hat{T}\right)\exp\left(-\tau\hat{V}\right)\right]$$

with Trotter-Suzuki decomposition

$$\mathrm{e}^{-\beta(\hat{T}+\hat{V})} = \prod^{N_\tau}\mathrm{e}^{-\tau(\hat{T}+\hat{V})} \simeq \prod^{N_\tau}\left(\mathrm{e}^{-\tau\hat{T}/2}\mathrm{e}^{-\tau\hat{V}}\mathrm{e}^{-\tau\hat{T}/2}\right)$$

Automated-algebra method

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Expression to evaluate

$$Q_N = \mathrm{tr}_N \left[\prod^{N_\tau} \exp\left(-\tau \hat{T}\right) \exp\left(-\tau \hat{V}\right) \right]$$

In momentum space

$$Q_N = \sum_{\mathbf{P}^{(1)}} \left\langle \mathbf{P}^{(1)} \middle| \prod_{N_\tau} \exp\left(-\tau \hat{T}\right) \exp\left(-\tau \hat{V}\right) \middle| \mathbf{P}^{(1)} \right\rangle$$

Inserting complete sets for each time slice

$$Q_N = \sum_{\{\mathbf{P}\}} \epsilon[\mathbf{P}^{(1)}]\epsilon[\mathbf{P}^{(2)}]\cdots\epsilon[\mathbf{P}^{(N_\tau)}]$$
$$\times V[\mathbf{P}^{(1)}, \mathbf{P}^{(2)}]V[\mathbf{P}^{(2)}, \mathbf{P}^{(3)}]\cdots V[\mathbf{P}^{(N_\tau)}, \mathbf{P}^{(1)}]$$

$$\boxed{\epsilon(p) = \mathrm{e}^{\frac{-\tau p^2}{2m}}}$$

Automated-algebra method

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Expression to evaluate

$$Q_N = \sum_{\{\mathbf{P}\}} \epsilon[\mathbf{P}^{(1)}]\epsilon[\mathbf{P}^{(2)}]\cdots\epsilon[\mathbf{P}^{(N_\tau)}] \times V[\mathbf{P}^{(1)},\mathbf{P}^{(2)}]V[\mathbf{P}^{(2)},\mathbf{P}^{(3)}]\cdots V[\mathbf{P}^{(N_\tau)},\mathbf{P}^{(1)}]$$

$$\begin{aligned} V[\mathbf{P}^{(i)},\mathbf{P}^{(j)}] &= \left\langle \mathbf{P}^{(i)} \middle| \exp\left(-\tau\hat{V}\right) \middle| \mathbf{P}^{(j)} \right\rangle \\ &= 1 + C f_1(\mathbf{P}^{(i)},\mathbf{P}^{(j)}) + C^2 f_2(\mathbf{P}^{(i)},\mathbf{P}^{(j)}) + \cdots \end{aligned}$$

$$\boxed{C = \exp(\tau g) - 1}$$

Example of f_n function in (2+2) system:

$$\begin{aligned} f_1(\mathbf{P},\mathbf{Q}) = {} & \delta_{p_1+p_3,q_1+q_3}\delta_{p_2,q_2}\delta_{p_4,q_4} + \delta_{p_2+p_3,q_2+q_3}\delta_{p_1,q_1}\delta_{p_4,q_4} \\ & + \delta_{p_1+p_4,q_2+q_4}\delta_{p_2,q_2}\delta_{p_3,q_3} + \delta_{p_2+p_4,q_2+q_4}\delta_{p_1,q_1}\delta_{p_3,q_3} \end{aligned}$$

$$f_2(\mathbf{P},\mathbf{Q}) = \delta_{p_1+p_3,q_1+q_3}\delta_{p_2+p_4,q_2+q_4} + \delta_{p_1+p_4,q_1+q_4}\delta_{p_2+p_3,q_2+q_3}$$

Automated-algebra method

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Expression to evaluate

$$Q_N = Q_N^{(0)} + C Q_N^{(1)} + C^2 Q_N^{(2)} + \cdots + C^{l_{\max}} Q_N^{(l_{\max})}$$

where each $Q_N^{(l)}$ contains only Gaussian and delta functions, and $l_{\max}$ is capped by N_τ and $\min(M, J)$

After "crunching" the δ-function from potential terms, the l^{th}-order coefficient is the summation of terms of the form

$$Q_N^{(l)} = \sum_{\{\mathbf{P}'\}} \epsilon[\mathbf{P}'^{(1)}] \epsilon[\mathbf{P}'^{(2)}] \cdots$$

Taking the continuum limit $\sum_k \to \left(\frac{L}{2\pi}\right)^d \int \mathrm{d}^d k$, every term is converted to a multidimensional Gaussian integral

$$\int \mathcal{D}\mathbf{x} \exp\left(-\frac{1}{2}\mathbf{x}^T \mathcal{A} \mathbf{x}\right) = \sqrt{\frac{(2\pi)^n}{\det \mathcal{A}}}$$

“AAll” in one diagram

$$Q_N = \mathrm{tr}_N\left[\exp\left(-\beta\hat{H}\right)\right]$$

$\det \mathcal{A}_1$ $\det \mathcal{A}_2$ $\det \mathcal{A}_3$ $\det \mathcal{A}_4$ $\det \mathcal{A}_5$

"AAll" in one diagram

$$Q_N = \mathrm{tr}_N \left[\exp\left(-\beta \hat{H}\right)\right]$$

- AA $\approx$ a symbolic calculator $\approx$ "poor man's (much more specialized) Mathematica"
- Unlike noodles, all the final expressions are independent of each other, affinity to scalable parallelization

$\det \mathcal{A}_1$ $\det \mathcal{A}_2$ $\det \mathcal{A}_3$ $\det \mathcal{A}_4$ $\det \mathcal{A}_5$

Automated-algebra method

Extra steps to Δb_n

- Volume Cancellation (Analytical)
  Recall the relation of b_n and Q_N,

$$\Delta b_3 = \frac{\Delta Q_3}{Q_1} - Q_1 \Delta b_2$$

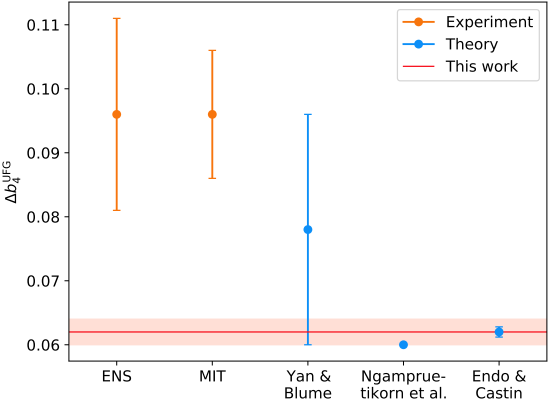
- Renormalization
  C is the new "bare coupling", which needs to be renormalized to the desired two-body physics, encoded by Δb_2
- Large-N_τ Extrapolation
  Extrapolate Δb_n to the $N_\tau \to \infty$ limit

RESULTS: HOMOGENEOUS SYSTEM AT UNITARITY

Overview

- Estimates of Δb_n up to $n = 5$ (or maybe a few extras)
- Observables
  - polarized and unpolarized systems
  - Pressure / Density / Compressibility / Susceptibility

Estimations of Δb_4 at unitarity



Orange	Experiment
Blue	Theory
Red	Our results

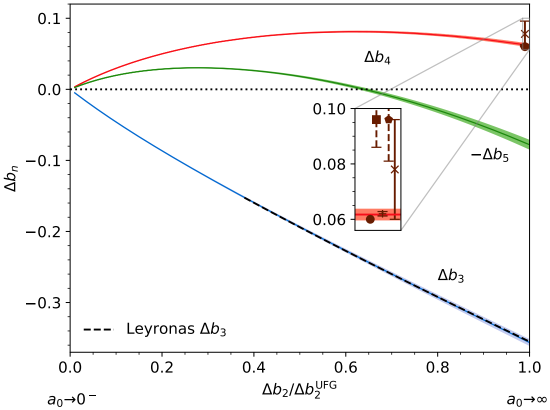
Yan and Blume
Phys. Rev. Lett. **116**, 230401 (2016)

Ngampruetikorn et al.
Phys. Rev. A **91**, 013606 (2015)

Endo and Castin
J. Phys. A Math. Theor. **49**(26), 265301 (2016)

Ku *et al.*
Science **335**, 6068, 563 (2012)

Estimations of Δb_n



Hou and Drut
Phys. Rev. Lett. **125**, 050403 (2020)

Wholespace contributions

- Nonmonotonic Δb_4 and Δb_5
- Similar magnitude of $|\Delta b_4|$ and $|\Delta b_5|$

Yan and Blume
Phys. Rev. Lett. **116**, 230401 (2016)

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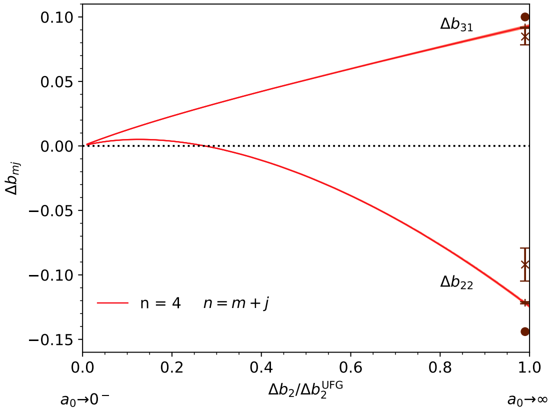

Hou and Drut
Phys. Rev. Lett. **125**, 050403 (2020)

Subspace breakdown

$$\Delta b_4 = 2\Delta b_{31} + \Delta b_{22}$$

Yan and Blume
Phys. Rev. Lett. **116**, 230401 (2016)

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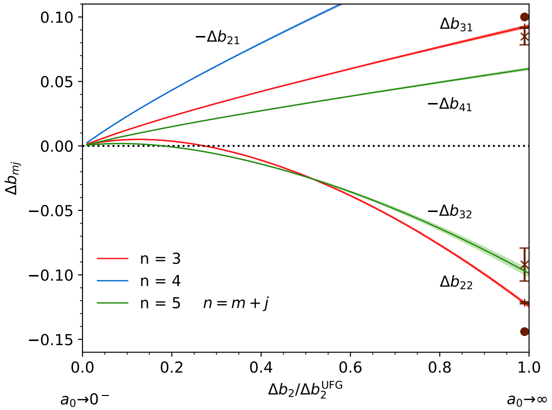

Hou and Drut
Phys. Rev. Lett. **125**, 050403 (2020)

Subspace breakdown

- Subspace sequences
  polaron Δb_{m1} / Δb_{m2}
  alternating sign
  more monotonic
- Subspace competitions
- Insights to future conjectures

Yan and Blume
Phys. Rev. Lett. **116**, 230401 (2016)

Ngampruetikorn et al.
Phys. Rev. A **91**, 013606 (2015)

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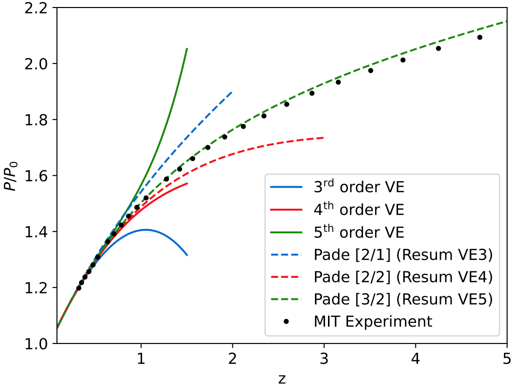
Phys. Rev. A **84**, 053633 (2011)

Pressure at unitarity



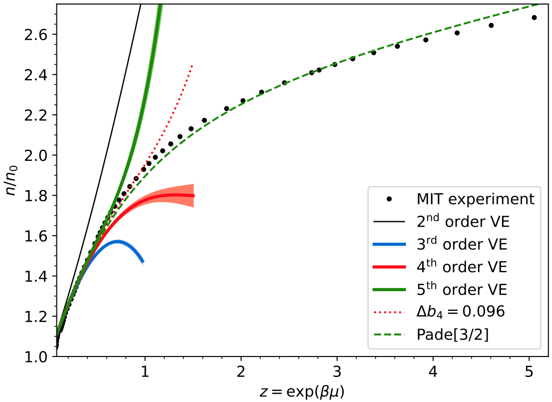
Pressure $P = P_0 + \Delta P$ compared with experimental determination

$$\Delta P = \frac{2}{\lambda_T^3} \sum_{n=2}^{\infty} \Delta b_n z^n$$

- Higher-order corrections are not "too" negligible
- Resummation methods show excellent agreement at large fugacity

Ku et al.
Science 335, 6068, 563 (2012)

Density at unitarity



Density $n = n_0 + \Delta n$ compared with experimental determination

$$\Delta n = \frac{2}{\lambda_T^3} \sum_{k=2}^{\infty} k \Delta b_k z^k$$

Hou and Drut
Phys. Rev. Lett. **125**, 050403 (2020)

Mukherjee et al.
Phys. Rev. Lett. **122**, 203402 (2019)

Density at unitarity - Zoom-in

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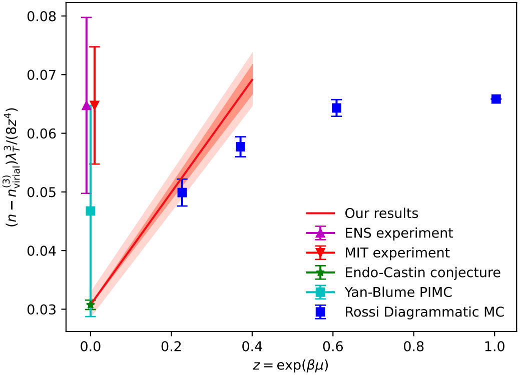


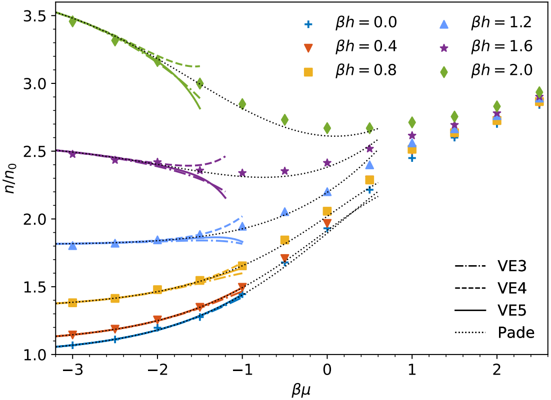
Zoom in higher-order contribution to the density

- Linear relation: $\Delta b_4 + \Delta b_5 \cdot z$
- Non-linear relation: higher-order contribution is required

Inner dark red: Uncertainty in slope (Δb_5) only
Outer light red: Uncertainties in both intercept (Δb_4) and slope (Δb_5)

Rossi et al.
Phys. Rev. Lett. **121**, 130405 (2018)

Density in polarized system



Density for each species

$$\Delta n_\uparrow = \frac{2}{\lambda_T^3} \sum_{n=2}^{\infty} \sum_{m+j=n} m z_\uparrow^m z_\downarrow^j \Delta b_{mj}$$

$$\Delta n_\downarrow = \frac{2}{\lambda_T^3} \sum_{n=2}^{\infty} \sum_{m+j=n} j z_\uparrow^m z_\downarrow^j \Delta b_{mj}$$

Usually express $z_\uparrow$ and $z_\downarrow$ in terms of $z = \exp(\beta\mu)$ and $\exp(\beta h)$, where

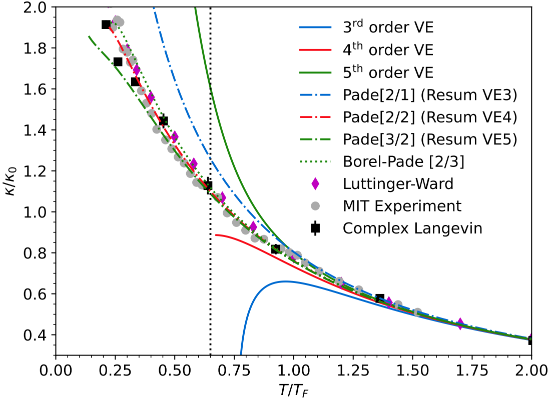
$$\mu = (\mu_\uparrow + \mu_\downarrow)/2$$

$$h = (\mu_\uparrow - \mu_\downarrow)/2$$

Hou and Drut
Phys. Rev. A **102**, 033319 (2020)

Rammelmuller et al.
Phys. Rev. Lett. **121**, 173001 (2018)

Compressibility



Hou and Drut
Phys. Rev. A **102**, 033319 (2020)

$$\kappa = -\frac{1}{V}\left[\frac{\partial V}{\partial P}\right]_T = \frac{\beta}{n^2}\left[\frac{\partial n}{\partial \beta\mu}\right]_T$$

where the derivative

$$\frac{\partial \Delta n}{\partial(\beta\mu)} = \sum_{m=2}^{\infty} m^2 \sum_{ij} \Delta b_{ij} z_\uparrow^i z_\downarrow^j$$

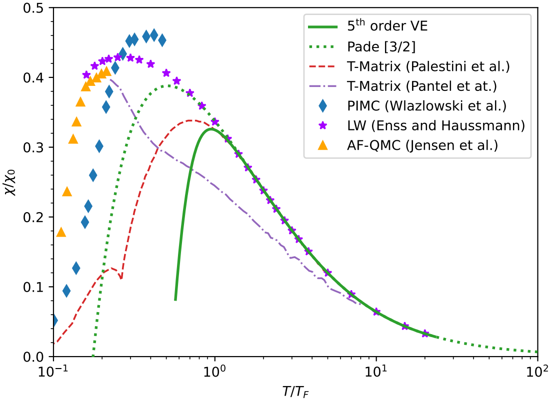
$$\kappa_0 = 3/(2n\epsilon_F)$$

Ku et al.
Science **335**, 563 (2012)

Enss and Haussmann
Phys. Rev. Lett. **109**, 195303 (2012)

Rammelmuller et al.
Phys. Rev. Lett. **121**, 173001 (2018)

Spin susceptibility - $\beta h = 0$

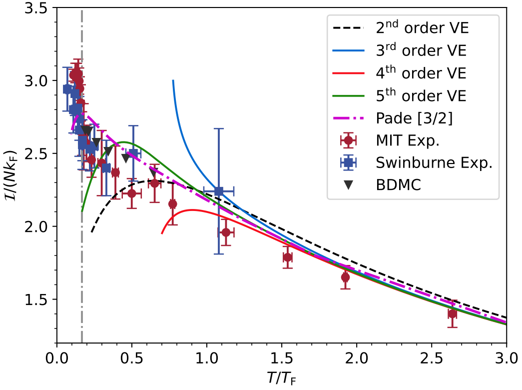


Spin susceptibility

$$\Delta\chi = \frac{\lambda_T^2}{8\pi} Q_1 \sum_{n=3}^{\infty} \sum_{mj} (m-j)^2 \Delta b_{mj} z_\uparrow^m z_\downarrow^j$$

$$\chi_0 = 3n/(2\epsilon_F)$$

Tan Contact at unitarity



Hou and Drut
Phys. Rev. Lett. **125**, 050403 (2020)

Tan Contact compared with experimental determinations

$$\mathcal{I} = \frac{8\pi^2}{\lambda_T} Q_1 \sum_{m=2}^{\infty} c_m z^m$$

$$c_m = \frac{1}{\sqrt{2\pi}} \frac{\partial \Delta b_m}{\partial \lambda}$$

where $\lambda = \sqrt{\beta}/a_s$.

Carcy et al.
Phys. Rev. Lett. **122**, 203401 (2019)

Mukherjee et al.
Phys. Rev. Lett. **122**, 203402 (2019)

Rossi et al.
Phys. Rev. Lett. **121**, 130406 (2018)

Summary

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Calculation of Δb_n [1]

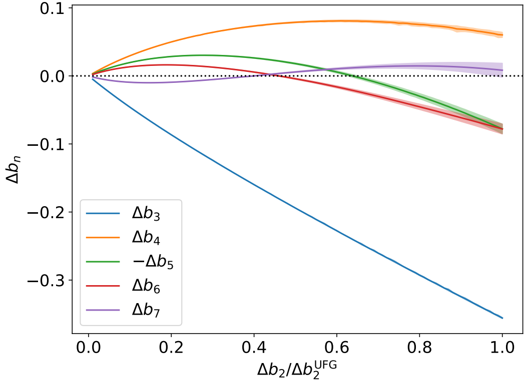
- Δb_3: agreement with existing numerical results
- Δb_4: resolved long-standing debate
- Δb_5: first-time prediction

Application of Δb_n [2] (with resummation)

- non-negligible higher-order contribution
- significant improvement with resummation
- (empirical) insights into analytical properties

  radius of convergence, optimal truncated order, etc.

The journey has not yet finished (but nearly)



- Quantitatively confident estimations for Δb_6 and Δb_7
- Qualitatively confident estimations for Δb_8 and Δb_9

Preliminary results

The journey has not yet finished (but nearly)

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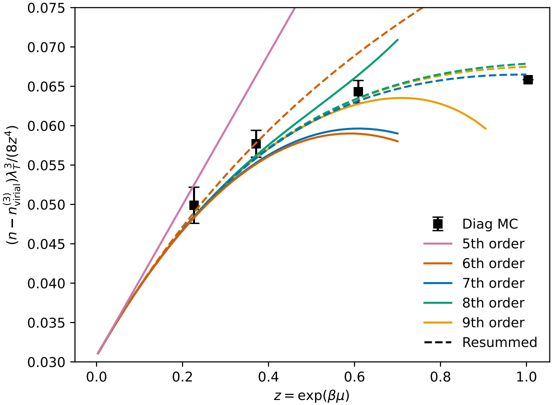
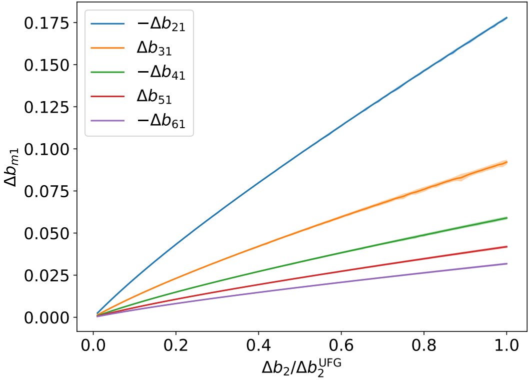


We found no significant improvements when including higher-order coefficients, possibly because

- Quantitative improvements are needed
- The resummation + QVE reaches the point of diminishing return
- Or anything could go wrong

Preliminary results

The short yet meaningful journey

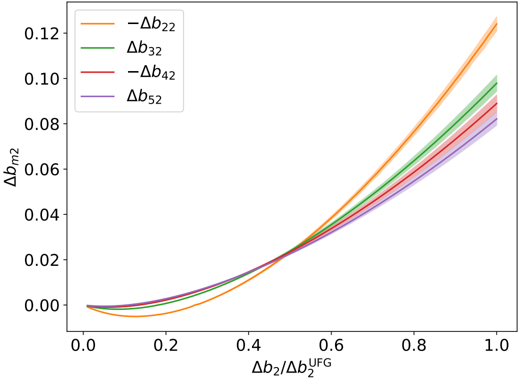


Preliminary results

The polaron sequence is in order just as usual

- Alternating sign
- Diminishing magnitude, i.e. approaching the non-interacting limit

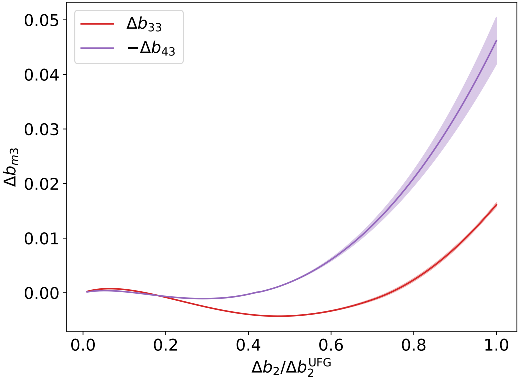
The short yet meaningful journey



The sequence Δb_{M2} shows similar features

Preliminary results

The short yet meaningful journey



The "sequence" of Δb_{M3} subspace is where things start to look more interesting

Preliminary results

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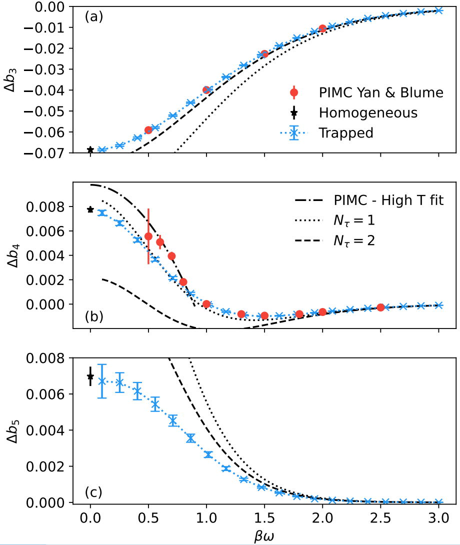
RESULTS: HARMONICALLY TRAPPED SYSTEM

Trapped Virial Coefficients - Wholespace



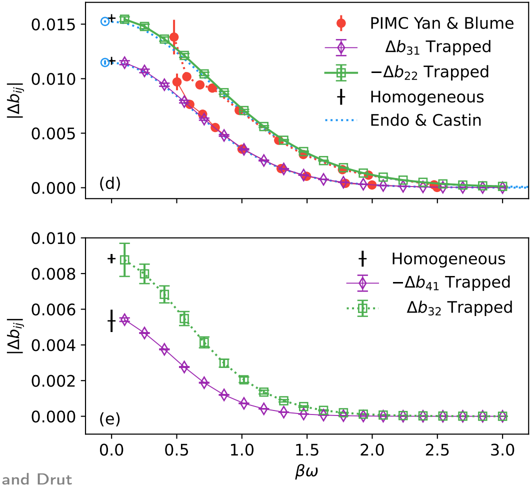
Δb_n^T at unitarity under external harmonic trapping

- Good agreement for Δb_3
- QMC suffers a sampling problem for Δb_4 at small $\beta\omega$, resulting in large uncertainty
- Analytic curves from the AA method

Hou and Drut
Phys. Rev. Res. 3, 033099(2021)

Yan and Blume
Phys. Rev. Lett. 116, 230401 (2016)

Trapped Virial Coefficients - Subspace



Hou and Drut
Phys. Rev. Res. 3, 033099(2021)

Δb_{ij}^{T} at unitarity under external harmonic trapping

- The polaron sequence
- Nearly collapse with the conjecture by Endo and Castin over all frequency

Endo and Castin
J. Phys. A Math. Theor. **49**(26), 265301 (2016)

Yan and Blume
Phys. Rev. Lett. **116**, 230401 (2016)

DISCUSSION AND OUTLOOK

Conclusions

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- The study of higher-order terms in the QVE is meaningful as they are not *that* negligible

  Our calculations at fifth (seventh) order is the first step in this direction

  Issue: computatonal cost

- With higher-order available and resummation methods, the QVE can be more than a benchmark method

  The analytic nature makes it ideal to explore unknown phenomena

  Issue 1: more systematic studies on resummation method

  Issue 2: correctness is not guaranteed *a priori*

- We may have reached / be very close to the point of diminishing return

Why is AA a good idea?

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- Results are analytical* functions of external parameters
- Continuum limit is taken immediately: no spatial extrapolation required
- No statistical sampling = No signal-to-noise issue = No Sign Problem
- Observables computation is straightforward: no source term required
- The computational cost becomes **very high** as N_τ increases

$(M!N!)^{N_\tau} \to (M!N!) \sum_{\{\mathbb{N}\}} \prod_{l_i \in \mathbb{N}} C_M^{l_i} C_N^{l_i}$ (Computaitonal cost for (3,3)-system, excluding the common factor $M!N!$)

N_τ	1	2	3	4	5	6	7	8
Num. of Terms	33	798	1.76E4	4.39E5	1.06E7	2.98E8	8.03E9	2.36E11

- Error estimation could be difficult: discretization error, extrapolation error from limited N_τ

New perspective

The combination of numerical and analytical fronts, pushing automated algebra as far as possible, may be a worthwhile research direction.

Outlook for AA method

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1. Generalize it to more general Hamiltonian and observables

   Neutron matter / Bose gas / Repulsive interaction

   Momentum distribution / correlation (e.g. structure factor) / time-dependent (e.g. quantum quench)

2. Further mathematical investigation

   Better understanding of resummations

   Incorporate symmetry to reduce computational cost

3. Technical improvement

   optimization / larger-scale parallel computation

4. Extension of the idea combining analytical and numerical computations

   Quantum Thermodynamics Computation Engine (QTCE)

THANK YOU

Resummation Method

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Idea

$$F(z) = \sum_{n}^{\infty} f_n z^n$$

With only the first few f_n known, is there a better approximation than the truncated series?

Resummation Method

Idea

$$F(z) = \sum_{n}^{\infty} f_n z^n$$

With only the first few f_n known, is there a better approximation than the truncated series?

Pade resummation

Pade approximant at order [M/N] with $M + N$ known coefficients

$$\widetilde{F}(z) = \frac{P_M(z)}{Q_N(z)} = \frac{p_0 + p_1 z + \cdots + p_M z^M}{1 + q_1 z + \cdots + q_N z^N}$$

Resummation Method

Borel transformation

$$\mathcal{B}F(z) = \sum_{n}^{\infty} \frac{f_n}{n!} z^n$$

$$B(z) \equiv \int_0^{\infty} \mathrm{d}t\ \mathrm{e}^{-t} \mathcal{B}F(tz) \to F(z)$$

Borel-Pade resummation

Apply Pade approximant to the series $\mathcal{B}F(z)$

$$B(z) = \int_0^{\infty} \mathrm{d}t \mathrm{e}^{-t} \frac{P_M(tz)}{Q_N(tz)},$$

Automated algebra - Working example

For a (1, 1)-system

$$Q_{11} = \sum_{\mathbf{p}_1\mathbf{p}_2} \langle \mathbf{p}_1\mathbf{p}_2 | e^{-\beta \hat{T}} e^{-\beta \hat{V}} | \mathbf{p}_1\mathbf{p}_2 \rangle$$
$$= \sum_{\mathbf{p}_1\mathbf{p}_2} e^{-\beta(p_1^2+p_2^2)/2m} \langle \mathbf{p}_1\mathbf{p}_2 | e^{-\beta \hat{V}} | \mathbf{p}_1\mathbf{p}_2 \rangle.$$

Inserting a complete sets, and the last term becomes

$$e^{-\beta \hat{V}} |\mathbf{x}_1\mathbf{x}_2\rangle = \prod_{\mathbf{z}} (1 + C\hat{n}_\uparrow(\mathbf{z})\hat{n}_\downarrow(\mathbf{z})) |\mathbf{x}_1\mathbf{x}_2\rangle$$
$$= |\mathbf{x}_1\mathbf{x}_2\rangle + C \sum_{\mathbf{z}} \delta_{\mathbf{x}_1,\mathbf{z}} \delta_{\mathbf{x}_2,\mathbf{z}} |\mathbf{x}_1\mathbf{x}_2\rangle$$
$$= \left[1 + C\delta_{\mathbf{x}_1,\mathbf{x}_2}\right] |\mathbf{x}_1\mathbf{x}_2\rangle,$$

where $C = (e^{\beta g} - 1)\ell^d$ is the "coupling strength" to be renormalized.

Automated algebra - Working example

The final result

$$\Delta Q_{11} = C \sum_{\mathbf{p}_1\mathbf{p}_2,\mathbf{x}_1\mathbf{x}_2} e^{-\beta(p_1^2+p_2^2)/2m} \delta_{\mathbf{x}_1,\mathbf{x}_2} |\langle \mathbf{x}_1\mathbf{x}_2|\mathbf{p}_1\mathbf{p}_2\rangle|^2,$$

In general case, we have

$$Q_{MN} = \sum_{\mathbf{P}_1\cdots\mathbf{P}_k} e^{-\tau\mathbf{P}_1^2/2m} \dots e^{-\tau\mathbf{P}_k^2/2m} \langle \mathbf{P}_1|e^{-\tau\hat{V}}|\mathbf{P}_2\rangle \cdots \langle \mathbf{P}_k|e^{-\tau\hat{V}}|\mathbf{P}_1\rangle$$

and the interaction term is

$$e^{-\beta\hat{V}} |\mathbf{X}\rangle = [1 + Cf_1(\mathbf{X}) + C^2 f_2(\mathbf{X}) + \ldots + C^{\min(M,N)} f_{\min(M,N)}(\mathbf{X})] |\mathbf{X}\rangle$$

where $f_i(\mathbf{X})$ is composed of a series of δ-functions.

Automated algebra - Technical details

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Computational Costs

- Complicity mainly comes from the interaction operator
- Roughly speaking, it increases sub-factorially $(M!N!)^{N_\tau}$
- Luckily, there are symmetries

Technical advantages

- Parallelization with high scalability
- Treat control parameters (dimension, trapping frequency, momentum, etc.) symbolically i.e. analytic smooth curve without repeating computations

Automated-algebra method revisited

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What it is

- A "symbolic calculator" to perform a limited set of algebraic operations
- An alternative/complementary to conventional statistical methods
- A parallelable method with nearly perfect scalability

What it is NOT

- Not a tool for any functions or operators

  "Yet Another Mathematica"
- Not a "user-friendly" method (for now)
- Not a tool only for the calculation of b_n

Comparison with stochastic methods

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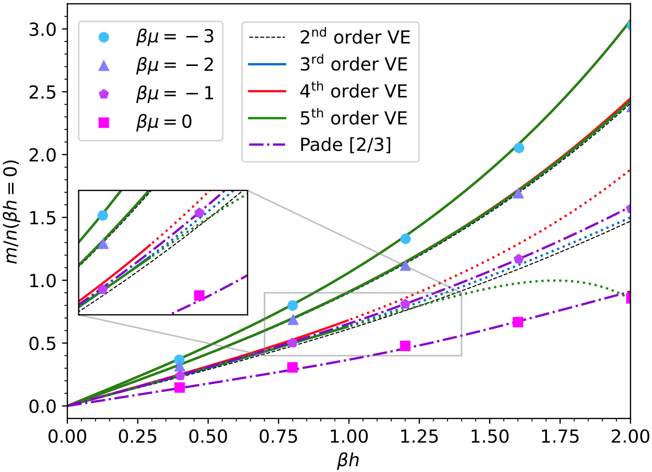
Automated algebra

- No statistical error, at expense of decomposition error (smaller N_τ and finite particle number)
- Symbolic parameters: results are analytic smooth function of d, ω, etc.
- Better scalability: each term is independent and easy to evaluate
  Open Science Grid
- Not applicable to lattice model as it relies on efficient Gaussian integral
- Renormalization: tuning $C = e^{\tau g} - 1$ on Δb_2
- Limited on specific interaction types (for now)

Magnetization



$$m = n_\uparrow - n_\downarrow$$

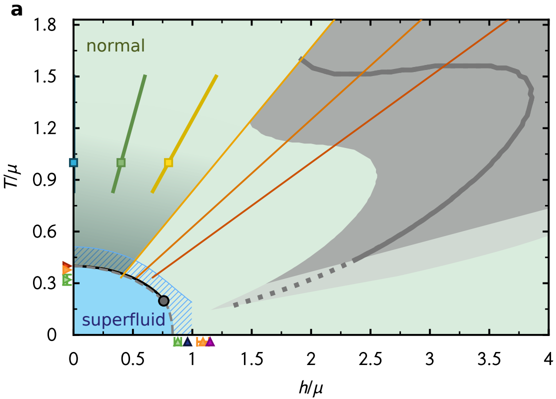
Dimensionless magnetization compared with QMC calculations

- Truncated results diverge as for $\beta\mu = -1$ and 0
- Resummed results shows nearly perfect agreements in both cases

Rammelmuller et al.
Phys. Rev. Lett. **121**, 173001 (2018)

The search of pseudogap

The suppression of spin susceptibility is an indicator of the pairing phase



Rammelmüller, Hou, Drut and Braun
Phys. Rev. A **103**, 043330 (2021)

The search of pseudogap

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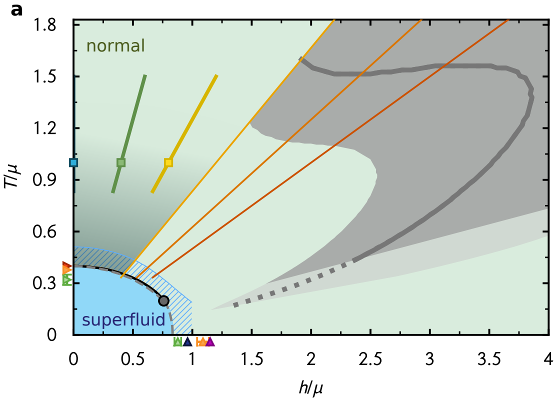
The suppression of spin susceptibility is an indicator of the pairing phase



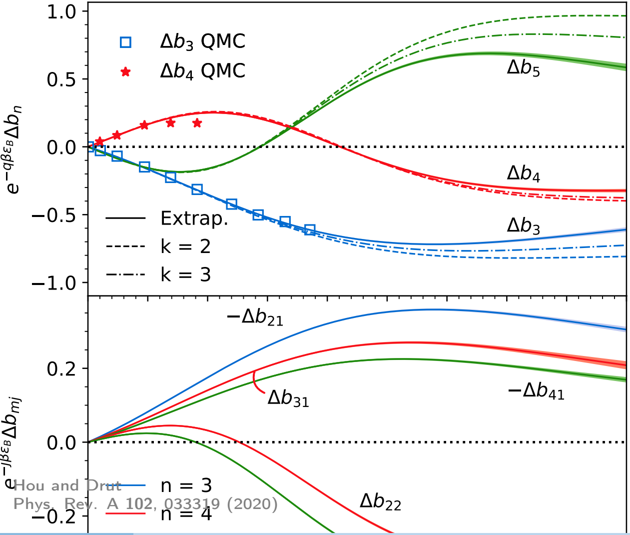
Claim

With the analytic expressions, we can obtain the smooth curve in unknown regimes with no extra computational costs.

Rammelmüller, Hou, Drut and Braun
Phys. Rev. A 103, 043330 (2021)

RESULTS: HOMOGENEOUS SYSTEM IN GENERAL SETTINGS

1D System - Virial Coefficients



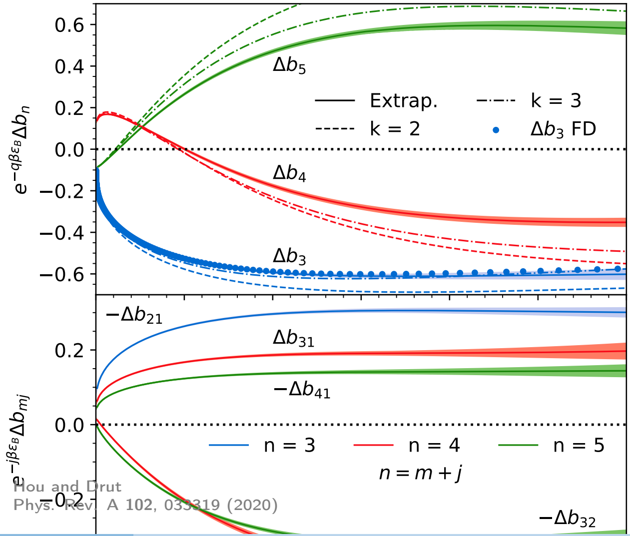
Hou and Drut
Phys. Rev. A 102, 033319 (2020)

Scaled virial coefficients as a function of physical coupling $\lambda_1 = (2\sqrt{\beta})/a_s$

- Polaron sequence in subspace
- Similar competitions

Hoffman et al.
Phys. Rev. A 91, 033618 (2015)

2D System - Virial Coefficients

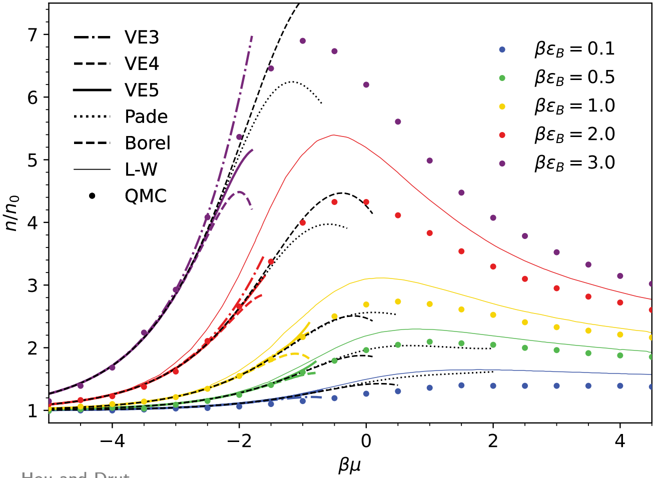


Hou and Drut
Phys. Rev. A 102, 033319 (2020)

Scaled virial coefficients as a function of physical coupling $\lambda_2^2 = \beta E_B$

Ngampruetikorn et al.
Phys. Rev. Lett 111, 265301 (2013)

2D System - Density



Hou and Drut
Phys. Rev. A **102**, 033319 (2020)

- The region of convergence is narrower compared to the 3D case
- The resummed results captures the qualitative behaviors

Bauer et al.
Phys. Rev. Lett. **112**, 135302 (2014)

Anderson and Drut
Phys. Rev. Lett. **115**, 115301 (2015)

Outlook for AA method

$$
\begin{aligned}
Q_n &= \mathrm{tr}_n[e^{-\beta \hat{H}}] \\
&= \sum_{\mathbf{P}} \langle \mathbf{P} | e^{-\tau \hat{T}} e^{-\tau \hat{V}} \cdots e^{-\tau \hat{T}} e^{-\tau \hat{V}} | \mathbf{P} \rangle
\end{aligned}
$$

Base Formula

- Original formulation for canonical partition function
- Suitable for homogeneous ultracold atoms

Outlook for AA method

$$
\begin{aligned}
Q_n &= \mathrm{tr}_n[e^{-\beta\hat{H}}] \\
&= \sum_{\mathbf{X}} \left\langle \boxed{\mathbf{X}} \middle| e^{-\tau\hat{H}_0} e^{-\tau\hat{V}} \cdots e^{-\tau\hat{H}_0} e^{-\tau\hat{V}} \middle| \boxed{\mathbf{X}} \right\rangle
\end{aligned}
$$

In coordinate representation

- Adapted to harmonically trapped ultracold atoms

Outlook for AA method

$$Q_n = \mathrm{tr}_n[e^{-\beta \hat{H}}]$$
$$= \sum_{\mathbf{P}} \langle \mathbf{P} | e^{-\tau \hat{T}} e^{-\tau \hat{V}} \cdots e^{-\tau \hat{T}} e^{-\tau \hat{V}} | \mathbf{P} \rangle$$

Different interactions

- Fermionic systems: SU(N) system / repulsive interaction

  Nishida and Son, Phys. Rev. A, 82, 043606 (2010)

- Bosonic systems: two- and three-body forces
- Spin-orbit coupling / p-wave interaction / ...

Outlook for AA method

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$$Q_n \left\langle \hat{O} \right\rangle = \mathrm{tr}_n[e^{-\beta \hat{H}} \hat{O}]$$
$$= \sum_{\mathbf{PQ}} \langle \mathbf{P} | (e^{-\tau \hat{T}} e^{-\tau \hat{V}})^k | \mathbf{Q} \rangle \; \langle \mathbf{Q} | \hat{O} | \mathbf{P} \rangle$$

Observables

- One-body operator: momentum distribution $\hat{n}(q)$

  Drut et al, Phys. Rev. Lett., **106**, 205302, (2011)

- Two-body operator: static structure factor $\sum_{\mathbf{r}} e^{-i\mathbf{q}\cdot\mathbf{r}} \hat{n}(\mathbf{r}) \hat{n}(0)$

  Alexandru et al, Phys. Rev. Lett., **126**, 132701 (2021)

Outlook for AA method

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$$Q_n \left\langle \hat{O} \right\rangle = \mathrm{tr}_n[e^{-\beta \hat{H}} \hat{O}]$$
$$= \sum_{\mathbf{PQ}} \langle \mathbf{P} | (e^{-\tau \hat{T}} e^{-\tau \hat{V}})^k | \mathbf{Q} \rangle \, \langle \mathbf{Q} | e^{it\hat{H}_1} \hat{O} e^{-it\hat{H}_1} | \mathbf{P} \rangle$$

Real-time evolution

- Quantum quench $\hat{H}_0 \to \hat{H}_0 + \Theta(t)\hat{H}_1$

  Sun et al. Phys. Rev. Lett., **125**, 110404 (2020)

- Dynamic structure factor $\sum_{\mathbf{r}} e^{-i(\mathbf{q}\cdot\mathbf{r} - \omega t)} \hat{n}(\mathbf{r}, t)\hat{n}(0,0)$

Outlook for AA method

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Conclusions / Claims about AA

- AA method has potential in more general settings
- The combination between numerical and analytical methods may be worth further investigations